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Analytical Approximate Solution of Chemical Kinetics Problems

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Abstract

In this article, the chemical kinetics problem is presented. The Differential Transformation Method (DTM) is presented to find an approximate analytical solution to the chemical kinetics problems. Proposed problem is system of nonlinear ordinary differential equations. We show converges analysis of the differential transform method. DTM applied to two examples. The method shows the form of fast converging series and the results prove the applicability of the proposed method, which gives accurate results.

Keywords: Chemical kinetic problems, Differential transform method, Power series, Approximate analytical solution.

1 | Introduction

In this paper we are concerned chemical kinetics problems system;

$$\begin{aligned}\frac{dx_1}{dt} &= -a_1x_1 + a_2x_2x_3, \\ \frac{dx_2}{dt} &= a_1x_1 - a_2x_2x_3 - a_3x_2^2, \\ \frac{dx_3}{dt} &= a_3x_2^2.\end{aligned}\tag{1}$$

With the initial conditions;

$$x_1(0) = 1, x_2(0) = 0, x_3(0) = 0.\tag{2}$$

Where a_1 , a_2 and a_3 are the reaction rates. In chemistry the chemical kinetics system is well described by nonlinear system of ordinary differential equations. Robertson [4] introduced the system in 1966, indicating the mathematical model of a chemical kinetic problem [1], [2].



Computational Algorithms and Numerical Dimensions.

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In recent years, numerous works have been focusing on the development of more advanced and efficient methods for the Homotopy Perturbation Method (HPM) and the Variation Iteration Method (VIM) [2], the picard-pade technique [3], the homotopy analysis method [3] and the Adomian's decomposition method [5] and iterative method [6]. The Differential Transformation Method (DTM) was first created by Zhou [7] to obtain approximate-analytical solutions to ordinary differential equations using Taylor series formulation. The differential transform method obtains an analytical solution in the form of a polynomial. It is different from the traditional high order Taylor's series method, which requires symbolic competition of the necessary derivatives of the data functions. The results of applying DTM to the chemical kinetics problems will be presented.

2 | Differential Transform Method

Differential transform of function $y(x)$ is defined as follows:

$$Y(k) = \frac{1}{k!} \left[\frac{d^k y(x)}{dx^k} \right]_{x=0}. \quad (3)$$

In Eq. (3), $y(x)$ is the original function and $Y(k)$ is the transformed function, which is called the T-function. Differential inverse transform of $Y(k)$ is defined as

$$y(x) = \sum_{k=0}^{\infty} x^k Y(k). \quad (4)$$

From Eq. (3) and (4), we obtain

$$y(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!} \left[\frac{d^k y(x)}{dx^k} \right]_{x=0}. \quad (5)$$

Eq. (5) implies that the concept of differential transform is derived from Taylor series expansion, but the method does not evaluate the derivatives symbolically.

However, relative derivatives are calculated by an iterative way which are described by the transformed equations of the original functions. In this study we use the lower case letter to represent the original function and upper case letter represent the transformed function.

From the definitions of Eqs. (2) and (4), it is easily proven that the transformed functions comply with the basic mathematics operations shown in Table 1.

In actual applications, the function $y(x)$ is expressed by a finite series and Eq. (4) can be written as:

$$y(x) = \sum_{k=0}^m x^k Y(k). \quad (6)$$

Eq. (5) implies that $\sum_{k=m+1}^{\infty} x^k Y(k)$, is negligibly small. In fact, m is decided by the convergence of natural frequency in this study.

Table 1. The fundamental operations of DTM.

Original Function	Transformed Function
$y(x) = u(x) \pm v(x)$	$Y(k) = U(k) \pm V(k)$
$y(x) = cw(x)$	$Y(k) = cW(k)$
$y(x) = dw/dx$	$Y(k) = (K+1)W(k+1)$
$y(x) = d^j w/dx^j$	$Y(k) = (K+1)(K+2) \dots (K+j)W(k+j)$
$y(x) = u(x)v(x)$	$Y(k) = \sum_{r=0}^k U(r)V(k-r)$

Theorem 1. If $y(x) = \exp(x)$ then $Y(k) = \frac{1}{k!}$.

Proof. By using Eq. (3), we have

$$W k) = \frac{1}{k!} \frac{\partial (e^x)}{\partial x^k} \Big|_{t=0} = \frac{1}{k!} e^x \Big|_{t=0} = \frac{1}{k!}.$$

Theorem 2. If $y(x) = \frac{\partial^m u(x)}{\partial x^m}$ then $Y(k) = \frac{(k+m)!}{k!} U(k+m)$.

Proof. By using Eq. (3), we have;

$$Y(k) = \frac{1}{k!} \frac{\partial^k}{\partial x^k} \frac{\partial^m u(x)}{\partial x^m} \Big|_{t=0} = \frac{1}{k!} \frac{\partial^{m+k} u(x)}{\partial x^{m+k}} \Big|_{t=0} = \frac{(k+m)!}{k!} U(k+m).$$

Theorem 3. If $y(x) = x^m$ then $k) = \delta(k-m) = \begin{cases} 1 & k=m \\ 0 & k \neq m \end{cases}$.

Proof. By using Eq. (3), we have;

$$W(k) = \frac{1}{k!} \frac{\partial (x^m)}{\partial x^k} \Big|_{t=0} = \begin{cases} \frac{1}{k!} \frac{\partial^k (x^k)}{\partial x^k} = \frac{k!}{k!} = 1, & k=m \\ \frac{1}{k!} \frac{\partial^k (x^m)}{\partial x^k} = 0, & k \neq m \end{cases}$$

Theorem 4. If $w(x) = \sin(wx + \alpha)$ then $W(k) = \frac{w^k}{k!} \sin\left(\frac{k\pi}{2} + \alpha\right)$.

Proof. By using Eq. (3), we have;

$$\begin{aligned} k=1 \quad W(1) &= \frac{1}{1!} \frac{\partial \sin(wx + \alpha)}{\partial x} \Big|_{x=0} = \frac{1}{1!} w \cos(wx + \alpha) \Big|_{x=0} = \frac{1}{1!} w \sin\left(\left(\frac{\pi}{2} + \alpha\right) + wx\right) \Big|_{x=0} \\ &= \frac{1}{1!} w \sin\left(\frac{\pi}{2} + \alpha\right), \\ k=2 \quad W(2) &= \frac{1}{2!} \frac{\partial^2 \sin(wx + \alpha)}{\partial x^2} \Big|_{x=0} = \frac{1}{2!} w^2 \cos\left(wx + \frac{\pi}{2} + \alpha\right) \Big|_{x=0} \\ &= \frac{1}{2!} w^2 \sin\left(\frac{\pi}{2} + \left(\frac{\pi}{2} + \alpha\right) + wx\right) \Big|_{x=0} = \frac{1}{2!} w^2 \sin\left(\frac{2\pi}{2} + \alpha + wx\right) \Big|_{x=0} = \frac{1}{2!} w^2 \sin\left(\frac{2\pi}{2} + \alpha\right). \end{aligned}$$

In the general form we have;

$$k=n \quad W(n) = \frac{1}{n!} \frac{\partial^n \sin(wx + \alpha)}{\partial x^n} \Big|_{x=0} = \frac{1}{n!} w^n \sin\left(wx + \frac{n\pi}{2} + \alpha\right) \Big|_{x=0} = \frac{1}{n!} w^n \sin\left(\frac{n\pi}{2} + \alpha\right).$$

Theorem 5. If $w(x) = \cos(wx + \alpha)$ then $W(k) = \frac{w^k}{k!} \cos\left(\frac{k\pi}{2} + \alpha\right)$.

Proof. By using Eq. (3), we have;

$$\begin{aligned} k=1 \quad W(1) &= \frac{1}{1!} \frac{\partial \cos(wx + \alpha)}{\partial x} \Big|_{x=0} = \frac{-1}{1!} w \sin(wx + \alpha) \Big|_{x=0} \\ &= \frac{1}{1!} w \cos\left(\left(\frac{\pi}{2} + \alpha\right) + wx\right) \Big|_{x=0} = \frac{1}{1!} w \cos\left(\frac{\pi}{2} + \alpha\right), \\ k=2 \quad W(2) &= \frac{1}{2!} \frac{\partial^2 \cos(wx + \alpha)}{\partial x^2} \Big|_{x=0} = \frac{-1}{2!} w^2 \sin\left(wx + \frac{\pi}{2} + \alpha\right) \Big|_{x=0} \\ &= \frac{1}{2!} w^2 \cos\left(\frac{\pi}{2} + \left(\frac{\pi}{2} + \alpha\right) + wx\right) \Big|_{x=0} = \frac{1}{2!} w^2 \cos\left(\frac{2\pi}{2} + \alpha + wx\right) \Big|_{x=0} = \frac{1}{2!} w^2 \cos\left(\frac{2\pi}{2} + \alpha\right). \end{aligned}$$

In the general form we have;

$$k=n \quad W(n) = \frac{1}{n!} \frac{\partial^n \cos(wx + \alpha)}{\partial x^n} \Big|_{x=0} = \frac{1}{n!} w^n \cos\left(wx + \frac{n\pi}{2} + \alpha\right) \Big|_{x=0} = \frac{1}{n!} w^n \cos\left(\frac{n\pi}{2} + \alpha\right).$$

In this part, we will show converges of the differential transform method to the exact solution by proof of some theorems [8].

Theorem 6. Consider the first order ordinary differential equation in here m, n are constants;

$$m \frac{dw(x)}{dx} + nw(x) = 0, w(0) = \gamma. \quad (7)$$



The differential transform method converges to the exact solution.

Proof. The general solution of differential equation is as $w(x) = \beta e^{-nx/m}$.

Now by taking the differential transform of Eq. (7), we have;

$$m W[K+1] + nW[K] = 0, W[0] = \beta.$$

We have $W[K+1] = \frac{-nW[K]}{m}$. By solve this recurrence relation, we get $W[K] = \frac{1}{k!} \left(\frac{-n}{m}\right)^k \beta$.

By using Eq. (8), the solution obtained by DTM is as follows:

$$w(x) = \beta \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{-nx}{m}\right)^k = \beta e^{-\frac{nx}{m}}. \quad (8)$$

Theorem 7. Consider the homogeneous ordinary differential equation of order n , where $v_i, i = 1, 2, \dots, n$ are variables;

$$v_0(x)w + \sum_{r=1}^n v_r(x) \frac{d^r w}{dx^r} = 0. \quad (9)$$

With initial conditions

$$w(x) = \beta_0, \left. \frac{d^i w}{dx^i} \right|_{x=0} = \beta_i, i = 1, 2, \dots, n-1. \quad (10)$$

The differential transform method converges to the exact solution.

Proof. By using with both Table 1 and the Eq. (9), we have;

$$\sum_{m=0}^k \left(V_0[k]W[k-m] + \sum_{r=1}^n \left[V_r[k] \left(\prod_{j=1}^r k-m+j \right) \right] W[k-m+r] \right) = 0.$$

From the initial conditions, we have;

$$W[0] = \beta_0, W[i] = \frac{\beta_i}{i!}, i = 1, 2, \dots, n-1.$$

By substituting the differential transforms, we have;

$$w(x) = \sum_{k=0}^{\infty} W[k]x^k, v_r(x) = \sum_{k=0}^{\infty} A_r[k]x^k.$$

Substituting the above formulas in Eq. (9), we get;

$$\begin{aligned} 0 &= \sum_{k=0}^{\infty} A_0[k]x^k \sum_{m=0}^{\infty} W[m]x^m + \sum_{r=1}^n \left(\sum_{k=0}^{\infty} A_r[k]x^k \cdot \left(\frac{d^r}{dx^r} \sum_{m=0}^{\infty} W[m]x^m \right) \right) \\ &= \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} A_0[m]W[k-m]x^k + \sum_{r=1}^n \left(\sum_{k=0}^{\infty} A_r[k]x^k \cdot \sum_{m=0}^{\infty} W[m+r] \right) \left(\prod_{j=1}^{r-1} m+j \right) x^k \\ &= \sum_{k=0}^{\infty} \sum_{m=0}^k \left(A_0[m]W[k-m] + \sum_{r=1}^n A_r[m]W[k-m+r] \left(\prod_{j=1}^r k-m+j \right) \right) x^k. \end{aligned}$$

We comparing coefficients and get;

$$\sum_{m=0}^k A_0[m]W[k-m] + \sum_{r=1}^n A_r[m]W[k-m+r] \left(\prod_{j=1}^r k-m+j \right) = 0.$$

3 | Numerical Example

Example 1. We consider the system of chemical kinetics;

$$\begin{aligned} \frac{dx_1}{dt} &= -a_1x_1 + a_2x_2x_3, \\ \frac{dx_2}{dt} &= a_3x_1 - a_4x_2x_3 - a_5x_2^2, \\ \frac{dx_3}{dt} &= a_6x_2^2. \end{aligned} \quad (11)$$

With the initial conditions

$$x_1(0) = 1, x_2(0) = 0, x_3(0) = 0. \quad (12)$$

When taking the one dimensional differential transform of Eq. (11), we can obtain:

$$\begin{aligned} X_1(n+1) &= \frac{1}{(n+1)} [-a_1 X_1(n) + a_2 \sum_{r=0}^n X_2(r) X_3(n-r)], \\ X_2(n+1) &= \frac{1}{(n+1)} [a_3 X_1(n) - a_4 \sum_{r=0}^n X_2(r) X_3(n-r) - a_5 \sum_{r=0}^n X_2(r) X_2(n-r)], \\ X_3(n+1) &= \frac{1}{(n+1)} [a_6 \sum_{r=0}^n X_2(r) X_2(n-r)], \end{aligned} \quad (13)$$

The initial conditions can be transformed at $x_0 = 0$, as;

$$X_1(0) = 1, X_2(0) = 0, X_3(0) = 0. \quad (14)$$

For $n = 0, 1, 2, \dots$, $X_1(n)$, $X_2(n)$, $X_3(n)$, coefficients can be calculated from Eqs. (13) and (14);

$$\begin{aligned} X_1(1) &= -a_1, X_2(1) = a_3, X_3(1) = 0, X_1(2) = \frac{a_1^2}{2}, \\ X_2(2) &= \frac{-a_3 a_1}{2}, X_3(2) = 0, X_1(3) = \frac{-a_1^3}{6}, \end{aligned} \quad (15)$$

$$\begin{aligned} X_2(3) &= \frac{1}{3} \left(\frac{a_3 a_1^2}{2} - a_5 a_3^2 \right), X_3(3) = \frac{a_6 a_3^2}{3}, \dots \end{aligned}$$

By using the inverse transformation rule for one dimensional in Eq. (6), the following solution can be obtained:

$$\begin{aligned} X_1(t) &= 1 - a_1 t + \frac{a_1^2}{2} t^2 - \frac{a_1^3}{6} t^3 + \dots, \\ X_2(t) &= a_3 t - \frac{a_3 a_1}{2} t^2 + \frac{1}{3} \left(\frac{a_3 a_1^2}{2} - a_5 a_3^2 \right) t^3 + \dots, \\ X_3(t) &= \frac{a_6 a_3^2}{3} t^3 + \dots \end{aligned} \quad (16)$$

Example 2. We consider the system of chemical kinetics;

$$\begin{aligned} \frac{dx_1}{dt} &= -x_1, \\ \frac{dx_2}{dt} &= x_1 - x_2^2, \\ \frac{dx_3}{dt} &= x_2^2. \end{aligned} \quad (17)$$

Subject to the initial conditions;

$$x_1(0) = 1, x_2(0) = 0, x_3(0) = 0. \quad (18)$$

When taking the one dimensional differential transform of Eqs. (17) and (18), we can obtain:

$$\begin{aligned} X_1(n+1) &= \frac{1}{(n+1)} [-X_1(n)], \\ X_2(n+1) &= \frac{1}{(n+1)} [X_1(n) - \sum_{r=0}^n X_2(r) X_2(n-r)], \\ X_3(n+1) &= \frac{1}{(n+1)} \left[\sum_{r=0}^n X_2(r) X_2(n-r) \right]. \end{aligned} \quad (19)$$

And

$$X_1(0) = 1, X_2(0) = 0, X_3(0) = 0. \quad (20)$$

For $n = 0, 1, 2, \dots$, $X_1(n)$, $X_2(n)$, $X_3(n)$, coefficients can be calculated from Eqs. (19) and (20).

$$\begin{aligned} x_1(1) &= -1, x_2(1) = 1, x_3(1) = 0, \\ x_1(2) &= \frac{1}{2}, x_2(2) = \frac{-1}{2}, x_3(2) = 0, \\ x_1(3) &= \frac{-1}{6}, x_2(3) = \frac{-1}{6}, x_3(3) = \frac{1}{3}. \end{aligned} \quad (21)$$

By using the inverse transformation rule for one dimensional in Eq. (6), the following solution can be obtained:

$$\begin{aligned}
 X_1(t) &= 1 - t + \frac{t^2}{2} - \frac{t^3}{6} + \frac{t^4}{24} - \dots, \\
 X_2(t) &= t - \frac{t^2}{2} + \frac{t^3}{6} + \frac{5t^4}{24} \dots, \\
 X_3(t) &= \frac{t^3}{3} - \frac{t^4}{4} + \dots.
 \end{aligned}
 \tag{22}$$

4 | Conclusion

In this study, the differential transform method is successfully expanded for the solution of chemical kinetics problems. Since the DTM gives rapidly converging series solutions, the differential transform method is more effective than other methods. Finally, all results prove the validity and efficiency of these methods in solving nonlinear differential equations.

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